



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:09 PM UTC

PDB ID : 2J6X / pdb_00002j6x
Title : The crystal structure of lactate oxidase
Authors : Leiros, I.; Wang, E.; Rasmussen, T.; Oksanen, E.; Repo, H.; Petersen, S.B.;
Heikinheimo, P.; Hough, E.
Deposited on : 2006-10-05
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

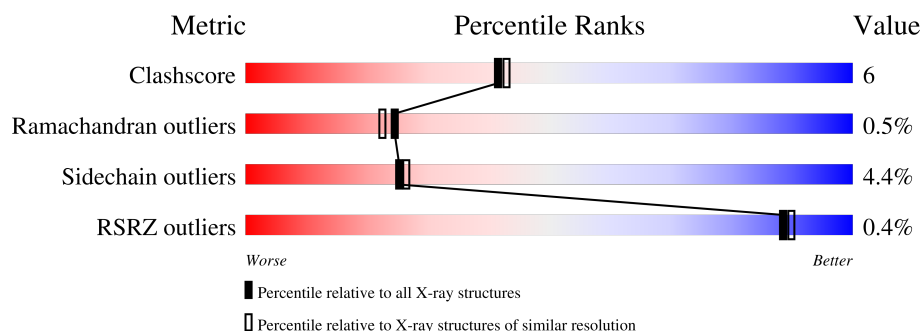
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	 84% 14% ..
1	B	374	 86% 10% ..
1	C	374	 84% 13% ..
1	D	374	 76% 17% • 6%
1	E	374	 80% 17% ..
1	F	374	 77% 16% • 5%

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Mol	Chain	Length	Quality of chain
1	G	374	84% 11%
1	H	374	82% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23895 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LACTATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2852	1802	493	550	7			
1	B	367	Total	C	N	O	S	0	0	0
			2827	1787	490	543	7			
1	C	368	Total	C	N	O	S	0	0	0
			2836	1792	491	546	7			
1	D	353	Total	C	N	O	S	0	0	0
			2717	1721	468	522	6			
1	E	367	Total	C	N	O	S	0	0	0
			2827	1787	490	543	7			
1	F	357	Total	C	N	O	S	0	0	0
			2748	1739	474	529	6			
1	G	367	Total	C	N	O	S	0	0	0
			2827	1787	490	543	7			
1	H	348	Total	C	N	O	S	0	0	0
			2682	1697	462	517	6			

There are 16 discrepancies between the modelled and reference sequences:

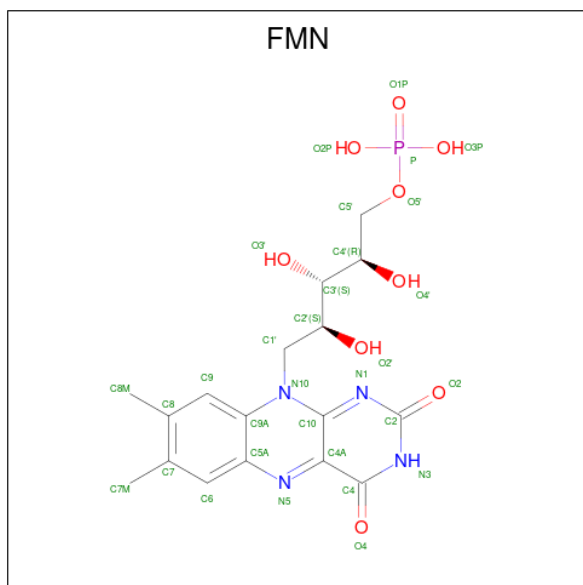
Chain	Residue	Modelled	Actual	Comment	Reference
A	232	ALA	GLY	conflict	UNP Q44467
A	255	ALA	ARG	conflict	UNP Q44467
B	232	ALA	GLY	conflict	UNP Q44467
B	255	ALA	ARG	conflict	UNP Q44467
C	232	ALA	GLY	conflict	UNP Q44467
C	255	ALA	ARG	conflict	UNP Q44467
D	232	ALA	GLY	conflict	UNP Q44467
D	255	ALA	ARG	conflict	UNP Q44467
E	232	ALA	GLY	conflict	UNP Q44467
E	255	ALA	ARG	conflict	UNP Q44467
F	232	ALA	GLY	conflict	UNP Q44467
F	255	ALA	ARG	conflict	UNP Q44467
G	232	ALA	GLY	conflict	UNP Q44467

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Chain	Residue	Modelled	Actual	Comment	Reference
G	255	ALA	ARG	conflict	UNP Q44467
H	232	ALA	GLY	conflict	UNP Q44467
H	255	ALA	ARG	conflict	UNP Q44467

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

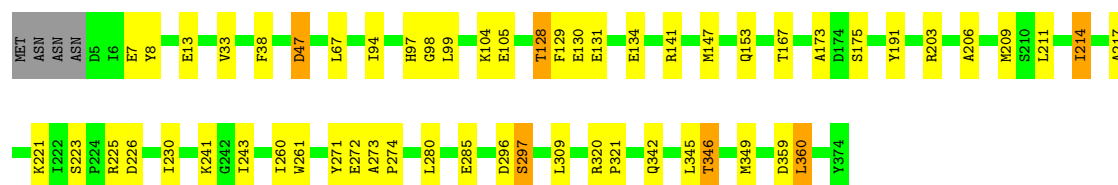
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		
4	B	185	Total	O	0	0
			185	185		
4	C	203	Total	O	0	0
			203	203		
4	D	145	Total	O	0	0
			145	145		
4	E	132	Total	O	0	0
			132	132		
4	F	148	Total	O	0	0
			148	148		
4	G	158	Total	O	0	0
			158	158		
4	H	160	Total	O	0	0
			160	160		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

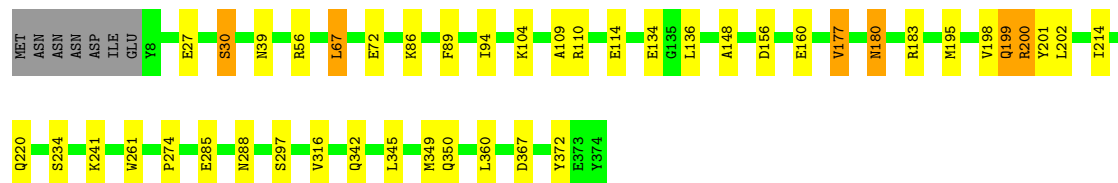
• Molecule 1: LACTATE OXIDASE

Chain A: 



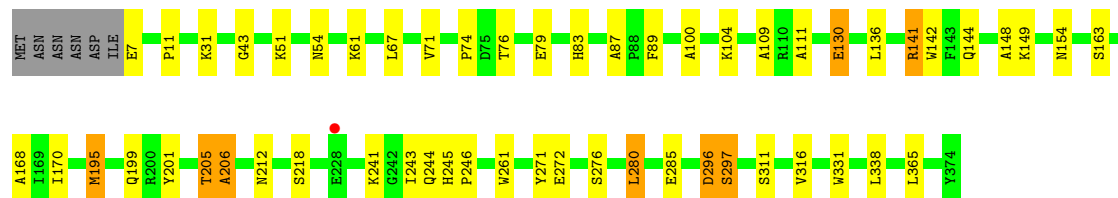
• Molecule 1: LACTATE OXIDASE

Chain B: 



• Molecule 1: LACTATE OXIDASE

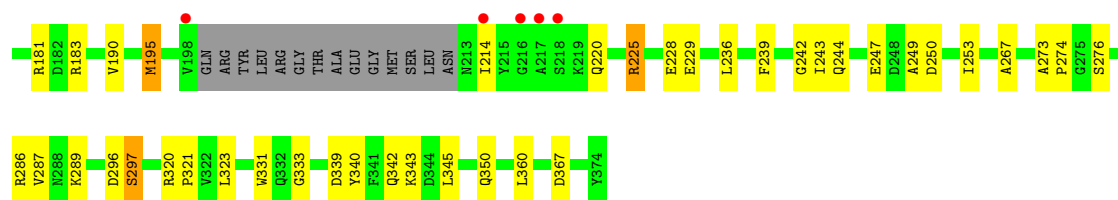
Chain C: 



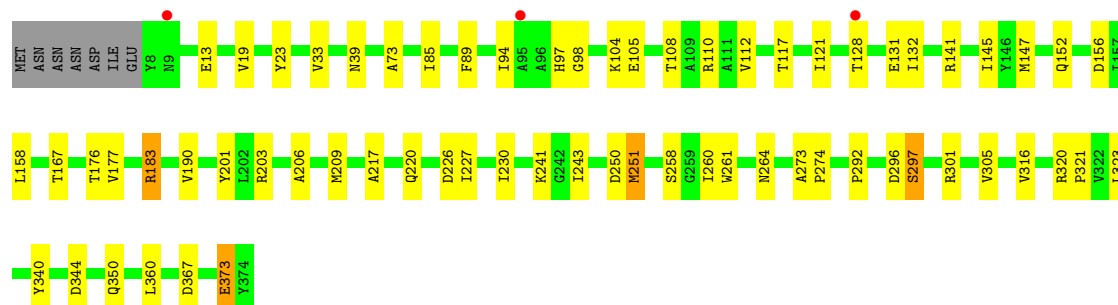
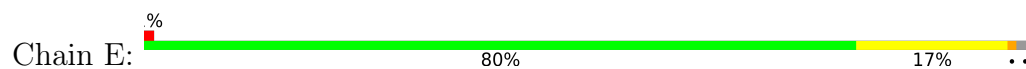
• Molecule 1: LACTATE OXIDASE

Chain D: 

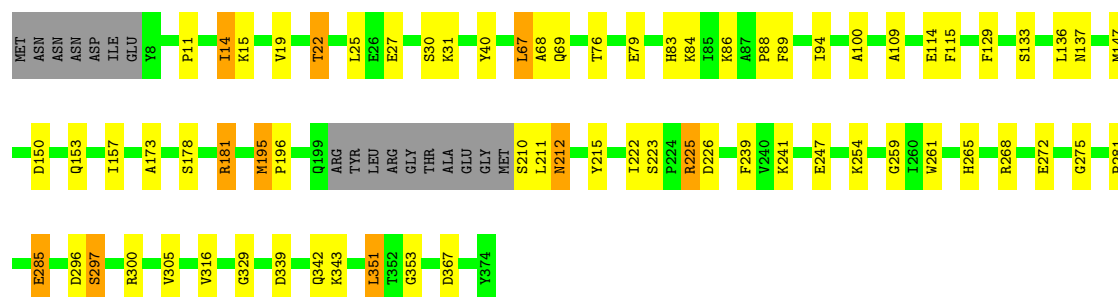




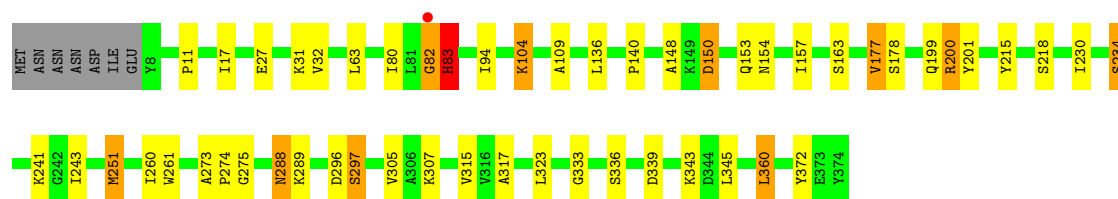
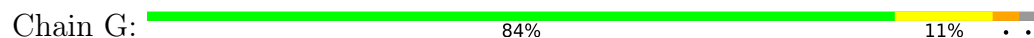
● Molecule 1: LACTATE OXIDASE



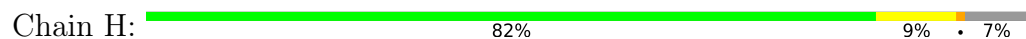
● Molecule 1: LACTATE OXIDASE

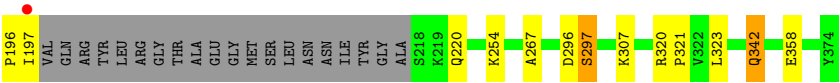


● Molecule 1: LACTATE OXIDASE



● Molecule 1: LACTATE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.34Å 134.74Å 185.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.10 12.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-2.10) 99.4 (12.00-2.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.257 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtrriage
Anisotropy	0.847	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23895	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3449e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/2916	0.94	4/3952 (0.1%)
1	B	0.65	0/2891	0.99	6/3918 (0.2%)
1	C	0.69	0/2900	0.95	4/3930 (0.1%)
1	D	0.67	0/2779	0.94	0/3767
1	E	0.63	0/2891	0.93	2/3918 (0.1%)
1	F	0.66	0/2810	0.94	3/3809 (0.1%)
1	G	0.66	0/2891	0.97	4/3918 (0.1%)
1	H	0.72	0/2743	0.96	3/3717 (0.1%)
All	All	0.67	0/22821	0.95	26/30929 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	GLN	N-CA-C	12.32	125.89	111.11
1	B	104	LYS	CB-CA-C	-8.01	106.25	115.79
1	B	199	GLN	CA-C-N	7.94	136.00	121.70
1	B	199	GLN	C-N-CA	7.94	136.00	121.70
1	A	130	GLU	N-CA-C	-7.85	102.74	113.18
1	B	195	MET	CA-C-N	7.07	126.90	119.05
1	B	195	MET	C-N-CA	7.07	126.90	119.05
1	E	33	VAL	CA-C-N	6.45	127.90	119.84
1	E	33	VAL	C-N-CA	6.45	127.90	119.84
1	C	104	LYS	CB-CA-C	-6.34	107.52	115.89
1	H	193	PHE	N-CA-C	6.32	120.80	112.72
1	C	43	GLY	N-CA-C	5.82	119.99	112.54
1	C	195	MET	CA-C-N	5.66	125.77	119.32
1	C	195	MET	C-N-CA	5.66	125.77	119.32
1	G	82	GLY	CA-C-N	5.65	131.87	121.70
1	G	82	GLY	C-N-CA	5.65	131.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LEU	CA-C-N	-5.56	112.87	119.05
1	A	280	LEU	C-N-CA	-5.56	112.87	119.05
1	A	94	ILE	N-CA-C	-5.46	101.14	108.35
1	F	195	MET	CA-C-N	5.26	125.31	119.32
1	F	195	MET	C-N-CA	5.26	125.31	119.32
1	G	275	GLY	N-CA-C	-5.25	105.22	111.36
1	G	372	TYR	N-CA-C	5.21	116.77	111.14
1	F	275	GLY	N-CA-C	-5.18	105.30	111.36
1	H	195	MET	CA-C-N	5.10	126.22	119.84
1	H	195	MET	C-N-CA	5.10	126.22	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2852	0	2779	45	0
1	B	2827	0	2758	28	0
1	C	2836	0	2764	35	0
1	D	2717	0	2648	45	0
1	E	2827	0	2758	44	0
1	F	2748	0	2678	39	0
1	G	2827	0	2758	39	0
1	H	2682	0	2611	23	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	1	0
2	F	31	0	19	0	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0
3	D	1	0	0	0	0
4	A	199	0	0	6	0
4	B	185	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	203	0	0	8	0
4	D	145	0	0	7	0
4	E	132	0	0	7	0
4	F	148	0	0	6	0
4	G	158	0	0	6	0
4	H	160	0	0	7	0
All	All	23895	0	21906	283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:MET:HE1	4:D:2070:HOH:O	1.42	1.20
1:F:40:TYR:O	1:F:268:ARG:NH2	1.82	1.10
1:C:141:ARG:HG2	1:C:141:ARG:HH11	1.24	0.99
1:A:209:MET:HE2	1:A:217:ALA:HB3	1.38	0.99
1:G:82:GLY:HA3	1:G:83:HIS:HB2	1.51	0.93
1:C:71:VAL:HG13	4:C:2190:HOH:O	1.71	0.90
1:B:180:ASN:HD22	1:B:180:ASN:H	1.19	0.90
1:C:71:VAL:CG1	4:C:2190:HOH:O	2.20	0.89
1:H:180:ASN:H	1:H:180:ASN:HD22	1.20	0.85
1:E:147:MET:HE3	1:E:226:ASP:HB3	1.58	0.85
1:G:82:GLY:HA3	1:G:83:HIS:CB	2.07	0.85
1:D:289:LYS:HD3	4:D:2102:HOH:O	1.75	0.84
1:E:39:ASN:HD22	1:E:183:ARG:HH11	1.25	0.84
1:A:129:PHE:O	1:A:129:PHE:CD2	2.31	0.84
1:H:94:ILE:HG21	1:H:323:LEU:HD21	1.62	0.81
1:G:148:ALA:H	1:G:154:ASN:HD21	1.25	0.81
1:D:50:THR:HG21	4:D:2093:HOH:O	1.81	0.81
1:H:128:THR:HG21	4:H:2072:HOH:O	1.81	0.81
1:D:273:ALA:HB3	4:D:2093:HOH:O	1.80	0.80
1:F:86:LYS:HD2	1:F:115:PHE:O	1.82	0.80
1:F:265:HIS:O	1:F:268:ARG:HG3	1.82	0.80
1:C:141:ARG:HG2	1:C:141:ARG:NH1	2.00	0.77
1:A:209:MET:HE2	1:A:217:ALA:CB	2.14	0.77
1:G:178:SER:HB3	1:G:215:TYR:HD1	1.51	0.76
1:D:19:VAL:CG2	1:D:340:TYR:HB2	2.16	0.75
1:E:209:MET:HE2	1:E:217:ALA:HB3	1.68	0.75
1:G:82:GLY:CA	1:G:83:HIS:HB2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:PRO:HG3	4:C:2190:HOH:O	1.88	0.73
1:D:19:VAL:HG21	1:D:340:TYR:HB2	1.71	0.72
1:B:39:ASN:HD22	1:B:183:ARG:HH11	1.37	0.71
1:A:209:MET:CE	1:A:217:ALA:HB3	2.17	0.70
1:D:104:LYS:HE2	4:D:2046:HOH:O	1.90	0.70
1:E:301:ARG:NH2	4:E:2106:HOH:O	2.24	0.69
1:B:27:GLU:O	1:B:30:SER:HB2	1.93	0.69
1:B:288:ASN:ND2	1:G:289:LYS:HD3	2.08	0.68
1:C:285:GLU:HG3	4:C:2160:HOH:O	1.93	0.68
1:D:118:ILE:HG22	1:D:140:PRO:HB2	1.76	0.68
1:B:156:ASP:O	1:B:160:GLU:HG3	1.94	0.68
1:G:178:SER:HB2	4:G:2079:HOH:O	1.93	0.68
1:D:128:THR:HB	4:D:2054:HOH:O	1.95	0.67
1:A:209:MET:CE	1:A:217:ALA:CB	2.73	0.67
1:B:200:ARG:HB2	4:B:2101:HOH:O	1.95	0.67
1:A:285:GLU:HG2	4:A:2153:HOH:O	1.96	0.65
1:E:121:ILE:HD12	1:E:132:ILE:HG21	1.79	0.65
1:F:247:GLU:HG3	4:F:2096:HOH:O	1.98	0.64
1:G:178:SER:CB	4:G:2079:HOH:O	2.46	0.64
1:F:27:GLU:O	1:F:30:SER:HB2	1.96	0.64
1:E:243:ILE:HD13	1:F:67:LEU:HD11	1.80	0.63
1:A:67:LEU:HD12	1:C:243:ILE:HD13	1.80	0.63
1:F:31:LYS:HE2	4:F:2008:HOH:O	1.97	0.63
1:F:211:LEU:O	1:F:212:ASN:HB2	1.98	0.63
1:H:83:HIS:CD2	4:H:2049:HOH:O	2.51	0.63
1:H:48:GLU:OE2	1:H:183:ARG:HD2	1.98	0.63
1:H:254:LYS:HD3	4:H:2111:HOH:O	1.99	0.63
1:E:243:ILE:HG13	1:E:260:ILE:HG23	1.82	0.62
1:A:241:LYS:NZ	4:A:2134:HOH:O	2.25	0.62
1:A:342:GLN:O	1:A:346:THR:HG23	1.99	0.62
1:E:350:GLN:NE2	4:E:2117:HOH:O	2.33	0.62
1:A:173:ALA:HB3	1:B:67:LEU:HD13	1.82	0.61
4:B:2138:HOH:O	1:G:288:ASN:HB3	1.99	0.61
1:G:82:GLY:HA3	1:G:83:HIS:CG	2.35	0.61
1:D:128:THR:HG23	1:D:131:GLU:H	1.64	0.61
1:E:39:ASN:ND2	1:E:183:ARG:HH11	1.99	0.60
1:H:44:ALA:HB1	1:H:267:ALA:O	2.01	0.60
1:F:79:GLU:HB3	1:F:84:LYS:HD2	1.84	0.59
1:B:285:GLU:HB3	4:B:2133:HOH:O	2.03	0.59
1:E:147:MET:HE1	1:E:230:ILE:HD11	1.84	0.59
1:G:148:ALA:HB2	1:G:201:TYR:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:HE1	1:A:230:ILE:HG13	1.84	0.59
1:G:218:SER:HB2	4:G:2096:HOH:O	2.03	0.58
1:D:345:LEU:HD11	1:D:360:LEU:HD11	1.85	0.58
1:A:47:ASP:HB2	1:A:271:TYR:OH	2.02	0.58
1:B:180:ASN:H	1:B:180:ASN:ND2	1.95	0.58
1:D:94:ILE:HG21	1:D:323:LEU:HD11	1.84	0.57
1:G:63:LEU:HG	1:G:307:LYS:HE2	1.86	0.57
1:F:210:SER:N	4:F:2079:HOH:O	2.37	0.57
1:G:273:ALA:HB1	1:G:274:PRO:HD2	1.87	0.57
1:E:147:MET:HE1	1:E:230:ILE:CD1	2.35	0.57
1:H:109:ALA:HB1	1:H:136:LEU:HG	1.85	0.57
1:H:358:GLU:HG2	4:H:2148:HOH:O	2.04	0.57
1:H:128:THR:HG23	1:H:131:GLU:H	1.70	0.56
1:A:128:THR:HG22	1:A:131:GLU:H	1.69	0.56
1:A:345:LEU:O	1:A:349:MET:HG3	2.06	0.56
1:F:223:SER:OG	1:F:225:ARG:HG3	2.05	0.56
1:G:83:HIS:CE1	1:G:140:PRO:HB3	2.40	0.56
1:F:76:THR:O	1:F:88:PRO:HD3	2.05	0.56
1:C:11:PRO:HG2	1:C:100:ALA:O	2.05	0.55
1:E:209:MET:HE2	1:E:217:ALA:CB	2.36	0.55
1:E:350:GLN:HG2	1:G:177:VAL:HB	1.87	0.55
1:C:195:MET:O	1:C:199:GLN:HG3	2.06	0.55
1:D:296:ASP:O	1:D:297:SER:HB2	2.07	0.55
1:B:198:VAL:C	1:B:200:ARG:HB3	2.31	0.55
1:G:109:ALA:HB1	1:G:136:LEU:HG	1.88	0.55
1:G:11:PRO:HB3	1:G:32:VAL:HG22	1.89	0.54
1:C:148:ALA:H	1:C:154:ASN:HD21	1.54	0.54
1:F:69:GLN:HG3	1:F:353:GLY:HA3	1.90	0.54
1:G:241:LYS:HA	1:G:261:TRP:HB3	1.89	0.54
1:H:63:LEU:HG	1:H:307:LYS:HE2	1.89	0.54
1:A:167:THR:HG22	4:A:2065:HOH:O	2.06	0.54
1:B:177:VAL:HB	1:D:350:GLN:HG2	1.89	0.54
1:D:296:ASP:OD1	1:D:296:ASP:C	2.51	0.53
1:G:345:LEU:HD11	1:G:360:LEU:HD21	1.91	0.53
1:H:296:ASP:O	1:H:297:SER:HB2	2.07	0.53
1:D:109:ALA:HB1	1:D:136:LEU:HG	1.91	0.53
1:E:94:ILE:HG23	2:E:1375:FMN:C6	2.39	0.53
1:C:241:LYS:HA	1:C:261:TRP:HB3	1.91	0.53
1:G:243:ILE:HD12	1:G:260:ILE:HG23	1.90	0.52
1:H:29:ALA:O	1:H:33:VAL:HG23	2.09	0.52
1:E:156:ASP:HB3	1:E:201:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ILE:HG12	1:D:333:GLY:HA2	1.92	0.52
1:D:19:VAL:HG21	1:D:340:TYR:CB	2.39	0.52
1:G:199:GLN:HG2	4:G:2089:HOH:O	2.10	0.52
1:A:273:ALA:HB1	1:A:274:PRO:HD2	1.90	0.52
1:G:296:ASP:HB3	1:G:317:ALA:HB3	1.92	0.52
1:A:296:ASP:O	1:A:297:SER:HB2	2.09	0.52
1:B:349:MET:HG2	1:B:360:LEU:HD21	1.91	0.52
1:D:19:VAL:HG23	1:D:340:TYR:CD1	2.45	0.52
1:G:80:ILE:O	1:G:83:HIS:HB2	2.10	0.52
1:F:14:ILE:HD11	4:F:2127:HOH:O	2.08	0.52
1:H:22:THR:O	1:H:25:LEU:HB2	2.10	0.52
1:F:296:ASP:O	1:F:297:SER:HB2	2.10	0.51
1:A:209:MET:HE3	1:A:217:ALA:HB1	1.92	0.51
1:F:241:LYS:NZ	4:F:2093:HOH:O	2.43	0.51
1:G:251:MET:C	1:G:251:MET:HE2	2.35	0.51
1:D:104:LYS:HG3	1:D:105:GLU:H	1.74	0.51
1:F:281:PRO:O	1:F:285:GLU:HG2	2.11	0.51
1:A:67:LEU:HD12	1:C:243:ILE:CD1	2.41	0.51
1:E:73:ALA:HA	4:E:2033:HOH:O	2.10	0.51
1:E:89:PHE:HA	1:E:316:VAL:O	2.10	0.51
1:E:128:THR:HG23	1:E:131:GLU:H	1.76	0.51
1:E:373:GLU:HB2	4:E:2130:HOH:O	2.11	0.51
1:G:230:ILE:O	1:G:234:SER:HB2	2.11	0.51
1:C:244:GLN:HE22	1:C:276:SER:HA	1.76	0.51
1:B:148:ALA:HB2	1:B:201:TYR:CD2	2.46	0.50
1:B:56:ARG:HG2	1:B:372:TYR:CD1	2.45	0.50
1:B:39:ASN:ND2	1:B:183:ARG:HH11	2.08	0.50
1:E:85:ILE:HG22	1:E:117:THR:HA	1.94	0.49
1:A:153:GLN:HE22	1:A:206:ALA:HB3	1.76	0.49
1:C:31:LYS:HE3	4:C:2019:HOH:O	2.11	0.49
1:D:113:SER:OG	1:D:136:LEU:O	2.23	0.49
1:G:150:ASP:OD2	1:G:153:GLN:NE2	2.32	0.49
1:C:67:LEU:HD13	1:D:173:ALA:HB3	1.95	0.49
1:E:190:VAL:HG22	4:E:2036:HOH:O	2.11	0.49
1:G:157:ILE:HD11	1:G:200:ARG:HD3	1.95	0.49
1:E:227:ILE:CD1	1:E:251:MET:HE1	2.43	0.48
1:A:243:ILE:HD12	1:A:260:ILE:HG23	1.96	0.48
1:D:249:ALA:O	1:D:253:ILE:HG12	2.13	0.48
1:G:150:ASP:HB2	4:G:2066:HOH:O	2.12	0.48
1:A:97:HIS:CD2	1:A:105:GLU:HG3	2.48	0.48
1:B:241:LYS:HA	1:B:261:TRP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ARG:NH1	4:F:2088:HOH:O	2.47	0.48
1:A:13:GLU:HB2	4:A:2171:HOH:O	2.12	0.48
1:A:129:PHE:O	1:A:129:PHE:CG	2.66	0.48
1:F:22:THR:HG22	1:F:300:ARG:HD2	1.96	0.48
1:H:296:ASP:OD1	1:H:296:ASP:C	2.56	0.48
1:A:241:LYS:HA	1:A:261:TRP:HB3	1.95	0.48
1:C:205:THR:HG21	4:C:2122:HOH:O	2.13	0.48
1:G:178:SER:HB3	1:G:215:TYR:CD1	2.39	0.48
1:B:199:GLN:O	1:B:202:LEU:HB2	2.14	0.48
1:E:206:ALA:O	1:E:209:MET:HB2	2.14	0.47
1:F:11:PRO:HD2	1:F:100:ALA:O	2.13	0.47
1:G:296:ASP:O	1:G:297:SER:HB2	2.14	0.47
1:E:147:MET:CE	1:E:230:ILE:HD11	2.44	0.47
1:A:206:ALA:HA	1:A:209:MET:HE3	1.96	0.47
1:D:339:ASP:OD2	1:D:343:LYS:HE2	2.14	0.47
1:E:296:ASP:C	1:E:296:ASP:OD1	2.58	0.47
1:F:129:PHE:O	1:F:133:SER:HB2	2.14	0.47
1:C:280:LEU:HD13	1:C:311:SER:HB2	1.95	0.47
1:E:97:HIS:CD2	1:E:105:GLU:HG3	2.50	0.47
1:F:241:LYS:HA	1:F:261:TRP:HB3	1.97	0.47
1:D:104:LYS:HD2	1:D:127:ALA:HB2	1.96	0.47
1:A:285:GLU:HG3	4:A:2150:HOH:O	2.15	0.47
1:D:195:MET:HE2	1:D:195:MET:HB3	1.75	0.47
1:E:108:THR:O	1:E:112:VAL:HG23	2.15	0.47
1:D:225:ARG:HA	1:D:228:GLU:HG2	1.96	0.46
1:A:345:LEU:HD11	1:A:360:LEU:HD21	1.95	0.46
1:D:76:THR:OG1	1:D:342:GLN:NE2	2.46	0.46
1:F:173:ALA:HB3	1:H:67:LEU:HD13	1.96	0.46
1:D:273:ALA:HB1	1:D:274:PRO:HD2	1.96	0.46
1:D:90:ILE:HG22	1:D:118:ILE:HG12	1.97	0.46
1:D:128:THR:HG22	1:D:131:GLU:OE1	2.15	0.46
1:D:225:ARG:NH2	1:D:229:GLU:OE2	2.48	0.46
1:E:340:TYR:O	1:E:344:ASP:HB2	2.16	0.46
1:C:205:THR:O	1:C:206:ALA:CB	2.64	0.45
1:C:296:ASP:O	1:C:297:SER:HB2	2.16	0.45
1:D:114:GLU:OE1	1:D:331:TRP:CZ3	2.69	0.45
1:H:180:ASN:H	1:H:180:ASN:ND2	1.99	0.45
1:A:221:LYS:HB2	1:B:72:GLU:HB2	1.97	0.45
1:E:176:THR:O	1:E:220:GLN:HG3	2.17	0.45
1:C:89:PHE:HA	1:C:316:VAL:O	2.17	0.45
1:D:79:GLU:OE2	1:D:82:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ASP:HB3	1:D:242:GLY:HA3	1.99	0.45
1:A:147:MET:HE3	1:A:226:ASP:HB3	1.98	0.45
1:B:350:GLN:NE2	4:B:2161:HOH:O	2.49	0.45
1:E:320:ARG:N	1:E:321:PRO:HD2	2.32	0.45
1:A:129:PHE:O	1:A:129:PHE:HD2	1.97	0.45
1:G:333:GLY:O	1:G:336:SER:HB2	2.16	0.44
1:G:27:GLU:OE2	1:G:31:LYS:HE2	2.17	0.44
1:A:342:GLN:O	1:A:346:THR:CG2	2.66	0.44
1:A:296:ASP:OD1	1:A:296:ASP:C	2.60	0.44
1:B:202:LEU:HD21	1:B:214:ILE:HG23	2.00	0.44
1:G:94:ILE:HG23	2:G:1375:FMN:C6	2.47	0.44
1:B:345:LEU:O	1:B:349:MET:HG3	2.17	0.44
1:F:241:LYS:HD2	1:F:261:TRP:CE2	2.53	0.44
1:G:148:ALA:N	1:G:154:ASN:HD21	2.02	0.44
1:H:125:SER:O	1:H:196:PRO:HD2	2.18	0.44
1:A:8:TYR:CE2	1:A:99:LEU:HA	2.53	0.44
1:A:359:ASP:OD2	1:F:254:LYS:NZ	2.50	0.44
1:B:274:PRO:HA	1:D:62:LEU:HD13	2.00	0.44
1:C:130:GLU:CD	1:C:130:GLU:H	2.26	0.44
1:F:222:ILE:HA	1:F:226:ASP:OD2	2.18	0.44
1:D:44:ALA:HB1	1:D:267:ALA:O	2.18	0.43
1:F:153:GLN:O	1:F:157:ILE:HG13	2.18	0.43
1:G:339:ASP:OD2	1:G:343:LYS:HE2	2.17	0.43
1:F:79:GLU:HA	1:F:83:HIS:O	2.18	0.43
1:B:110:ARG:O	1:B:114:GLU:HG3	2.18	0.43
1:G:104:LYS:HD3	4:G:2058:HOH:O	2.18	0.43
1:H:52:ARG:CD	4:H:2028:HOH:O	2.65	0.43
1:C:271:TYR:CE2	1:C:272:GLU:HG3	2.53	0.43
1:E:296:ASP:O	1:E:297:SER:HB2	2.17	0.43
1:D:104:LYS:HG3	1:D:105:GLU:N	2.34	0.43
1:D:320:ARG:N	1:D:321:PRO:HD2	2.34	0.43
1:H:52:ARG:HD2	4:H:2028:HOH:O	2.17	0.43
1:B:86:LYS:HD2	4:B:2063:HOH:O	2.18	0.43
1:C:148:ALA:HB2	1:C:201:TYR:CD2	2.53	0.43
1:E:251:MET:HE2	1:F:68:ALA:HB3	2.00	0.43
1:A:223:SER:OG	1:A:225:ARG:HG2	2.19	0.43
1:A:320:ARG:N	1:A:321:PRO:HD2	2.34	0.43
1:C:79:GLU:HA	1:C:83:HIS:O	2.19	0.43
1:D:128:THR:HG21	4:D:2055:HOH:O	2.19	0.43
1:E:177:VAL:HG12	1:F:351:LEU:CD1	2.48	0.43
1:C:142:TRP:CG	1:C:168:ALA:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASN:HB2	4:C:2127:HOH:O	2.18	0.43
1:E:98:GLY:CA	1:E:104:LYS:HG2	2.49	0.43
1:F:109:ALA:HB1	1:F:136:LEU:HG	2.01	0.43
1:F:339:ASP:OD2	1:F:343:LYS:HE2	2.19	0.43
1:C:109:ALA:HB1	1:C:136:LEU:HG	2.01	0.43
1:E:128:THR:HG21	4:E:2048:HOH:O	2.19	0.43
1:A:97:HIS:CG	1:A:105:GLU:HG3	2.53	0.42
1:C:245:HIS:HA	1:C:246:PRO:HD3	1.95	0.42
1:E:305:VAL:HG22	1:E:316:VAL:HG21	2.01	0.42
1:B:110:ARG:O	1:B:114:GLU:CG	2.67	0.42
1:H:320:ARG:N	1:H:321:PRO:HD2	2.34	0.42
1:C:51:LYS:NZ	4:C:2033:HOH:O	2.52	0.42
1:D:81:LEU:HD11	1:D:239:PHE:CE2	2.55	0.42
1:A:98:GLY:HA2	1:A:104:LYS:HG2	2.02	0.42
1:E:258:SER:O	1:E:292:PRO:HD2	2.19	0.42
1:G:148:ALA:H	1:G:154:ASN:ND2	2.05	0.42
1:E:145:ILE:HD11	1:E:230:ILE:HD13	2.02	0.42
1:E:273:ALA:HB1	1:E:274:PRO:HD2	2.00	0.42
1:D:244:GLN:HE22	1:D:276:SER:HA	1.85	0.41
1:H:342:GLN:NE2	4:H:2140:HOH:O	2.53	0.41
1:F:178:SER:HB2	1:F:215:TYR:HD1	1.85	0.41
1:F:305:VAL:HG22	1:F:316:VAL:HG21	2.02	0.41
1:A:191:TYR:CE1	1:A:211:LEU:HD12	2.54	0.41
1:C:51:LYS:O	1:C:54:ASN:HB2	2.20	0.41
1:C:61:LYS:HB3	1:C:365:LEU:HD13	2.02	0.41
1:C:144:GLN:HA	1:C:170:ILE:HB	2.02	0.41
1:G:305:VAL:HB	1:G:345:LEU:HD13	2.02	0.41
1:B:156:ASP:HB3	1:B:200:ARG:HH21	1.85	0.41
1:C:149:LYS:NZ	1:C:218:SER:O	2.54	0.41
1:D:162:LYS:HE3	1:D:236:LEU:HD21	2.01	0.41
1:E:264:ASN:HA	4:E:2058:HOH:O	2.20	0.41
1:H:176:THR:O	1:H:220:GLN:HG2	2.21	0.41
1:F:181:ARG:H	1:F:181:ARG:HG2	1.67	0.41
1:D:247:GLU:OE1	1:D:286:ARG:NH1	2.50	0.41
1:B:109:ALA:HB1	1:B:136:LEU:HG	2.03	0.41
1:F:195:MET:HA	1:F:196:PRO:HD2	1.87	0.41
1:A:342:GLN:HG3	4:A:2177:HOH:O	2.20	0.41
1:E:152:GLN:HB3	1:E:203:ARG:HH21	1.85	0.41
1:F:89:PHE:HA	1:F:316:VAL:O	2.20	0.41
1:C:111:ALA:HB2	1:C:331:TRP:O	2.20	0.41
1:B:89:PHE:HA	1:B:316:VAL:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:MET:CE	1:F:68:ALA:HB3	2.51	0.40
1:D:273:ALA:HB1	1:D:274:PRO:CD	2.52	0.40
1:A:33:VAL:HB	1:A:38:PHE:HB2	2.02	0.40
1:A:153:GLN:NE2	1:A:203:ARG:H	2.18	0.40
1:A:271:TYR:CG	1:A:272:GLU:N	2.89	0.40
1:C:76:THR:O	1:C:87:ALA:HA	2.22	0.40
1:E:241:LYS:HA	1:E:261:TRP:HB3	2.03	0.40
1:A:209:MET:SD	1:A:214:ILE:HG12	2.61	0.40
1:E:23:TYR:CE2	1:E:301:ARG:NH1	2.89	0.40
1:F:239:PHE:CE1	1:F:259:GLY:HA3	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/374 (98%)	359 (98%)	8 (2%)	1 (0%)	36	36
1	B	365/374 (98%)	352 (96%)	11 (3%)	2 (0%)	24	22
1	C	366/374 (98%)	352 (96%)	12 (3%)	2 (0%)	24	22
1	D	349/374 (93%)	338 (97%)	10 (3%)	1 (0%)	36	36
1	E	365/374 (98%)	351 (96%)	13 (4%)	1 (0%)	36	36
1	F	353/374 (94%)	339 (96%)	10 (3%)	4 (1%)	11	8
1	G	365/374 (98%)	350 (96%)	13 (4%)	2 (0%)	24	22
1	H	344/374 (92%)	335 (97%)	8 (2%)	1 (0%)	36	36
All	All	2875/2992 (96%)	2776 (97%)	85 (3%)	14 (0%)	24	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	200	ARG
1	B	297	SER
1	C	297	SER
1	D	297	SER
1	E	297	SER
1	F	297	SER
1	G	83	HIS
1	G	297	SER
1	H	297	SER
1	C	206	ALA
1	F	212	ASN
1	F	19	VAL
1	F	329	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/297 (99%)	283 (97%)	10 (3%)	32	35
1	B	290/297 (98%)	280 (97%)	10 (3%)	32	35
1	C	291/297 (98%)	283 (97%)	8 (3%)	39	45
1	D	279/297 (94%)	261 (94%)	18 (6%)	15	13
1	E	290/297 (98%)	277 (96%)	13 (4%)	24	25
1	F	283/297 (95%)	266 (94%)	17 (6%)	17	15
1	G	290/297 (98%)	277 (96%)	13 (4%)	24	25
1	H	276/297 (93%)	265 (96%)	11 (4%)	28	29
All	All	2292/2376 (96%)	2192 (96%)	100 (4%)	25	26

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	128	THR
1	A	134	GLU
1	A	141	ARG
1	A	175	SER
1	A	214	ILE
1	A	309	LEU
1	A	346	THR
1	A	360	LEU
1	B	30	SER
1	B	67	LEU
1	B	94	ILE
1	B	134	GLU
1	B	177	VAL
1	B	180	ASN
1	B	220	GLN
1	B	234	SER
1	B	342	GLN
1	B	367	ASP
1	C	7	GLU
1	C	130	GLU
1	C	141	ARG
1	C	163	SER
1	C	205	THR
1	C	280	LEU
1	C	296	ASP
1	C	338	LEU
1	D	20	VAL
1	D	113	SER
1	D	118	ILE
1	D	133	SER
1	D	134	GLU
1	D	141	ARG
1	D	160	GLU
1	D	181	ARG
1	D	183	ARG
1	D	190	VAL
1	D	195	MET
1	D	214	ILE
1	D	220	GLN
1	D	225	ARG
1	D	243	ILE
1	D	250	ASP

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Mol	Chain	Res	Type
1	D	287	VAL
1	D	367	ASP
1	E	13	GLU
1	E	19	VAL
1	E	110	ARG
1	E	141	ARG
1	E	158	LEU
1	E	167	THR
1	E	183	ARG
1	E	250	ASP
1	E	251	MET
1	E	323	LEU
1	E	360	LEU
1	E	367	ASP
1	E	373	GLU
1	F	14	ILE
1	F	15	LYS
1	F	22	THR
1	F	25	LEU
1	F	67	LEU
1	F	94	ILE
1	F	114	GLU
1	F	137	ASN
1	F	147	MET
1	F	150	ASP
1	F	181	ARG
1	F	225	ARG
1	F	272	GLU
1	F	285	GLU
1	F	342	GLN
1	F	351	LEU
1	F	367	ASP
1	G	17	ILE
1	G	83	HIS
1	G	104	LYS
1	G	150	ASP
1	G	163	SER
1	G	177	VAL
1	G	200	ARG
1	G	234	SER
1	G	251	MET
1	G	288	ASN

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Mol	Chain	Res	Type
1	G	315	VAL
1	G	323	LEU
1	G	360	LEU
1	H	25	LEU
1	H	32	VAL
1	H	52	ARG
1	H	80	ILE
1	H	134	GLU
1	H	145	ILE
1	H	153	GLN
1	H	167	THR
1	H	180	ASN
1	H	197	ILE
1	H	342	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	153	GLN
1	B	39	ASN
1	B	69	GLN
1	B	180	ASN
1	B	350	GLN
1	C	137	ASN
1	C	154	ASN
1	C	244	GLN
1	D	244	GLN
1	D	342	GLN
1	E	39	ASN
1	E	199	GLN
1	F	9	ASN
1	F	69	GLN
1	F	137	ASN
1	F	153	GLN
1	G	154	ASN
1	G	187	ASN
1	G	199	GLN
1	G	244	GLN
1	H	9	ASN
1	H	35	HIS
1	H	180	ASN

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Mol	Chain	Res	Type
1	H	187	ASN
1	H	245	HIS
1	H	350	GLN
1	H	356	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMN	H	1375	-	33,33,33	1.04	2 (6%)	48,50,50	1.20	6 (12%)
2	FMN	D	1375	-	33,33,33	1.07	2 (6%)	48,50,50	1.38	9 (18%)
2	FMN	A	1375	-	33,33,33	1.17	2 (6%)	48,50,50	1.23	7 (14%)
2	FMN	C	1375	-	33,33,33	1.15	2 (6%)	48,50,50	1.36	7 (14%)
2	FMN	B	1375	-	33,33,33	0.99	2 (6%)	48,50,50	1.32	5 (10%)
2	FMN	E	1375	-	33,33,33	1.03	2 (6%)	48,50,50	1.30	9 (18%)
2	FMN	G	1375	-	33,33,33	1.10	2 (6%)	48,50,50	1.09	4 (8%)
2	FMN	F	1375	-	33,33,33	1.05	2 (6%)	48,50,50	1.34	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	H	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	D	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	A	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	C	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	B	1375	-	-	4/18/18/18	0/3/3/3
2	FMN	E	1375	-	-	4/18/18/18	0/3/3/3
2	FMN	G	1375	-	-	1/18/18/18	0/3/3/3
2	FMN	F	1375	-	-	3/18/18/18	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1375	FMN	C4A-N5	4.06	1.39	1.30
2	C	1375	FMN	C4A-N5	3.90	1.39	1.30
2	D	1375	FMN	C4A-N5	3.72	1.38	1.30
2	E	1375	FMN	C4A-N5	3.66	1.38	1.30
2	H	1375	FMN	C4A-N5	3.53	1.38	1.30
2	B	1375	FMN	C4A-N5	3.50	1.38	1.30
2	G	1375	FMN	C4A-N5	3.47	1.38	1.30
2	G	1375	FMN	C10-N1	3.43	1.40	1.33
2	F	1375	FMN	C4A-N5	3.30	1.37	1.30
2	A	1375	FMN	C10-N1	3.21	1.39	1.33
2	C	1375	FMN	C10-N1	3.11	1.39	1.33
2	H	1375	FMN	C10-N1	2.91	1.39	1.33
2	D	1375	FMN	C10-N1	2.82	1.38	1.33
2	E	1375	FMN	C10-N1	2.74	1.38	1.33
2	F	1375	FMN	C10-N1	2.58	1.38	1.33
2	B	1375	FMN	C10-N1	2.18	1.37	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1375	FMN	C4A-C10-N10	3.38	121.32	116.48
2	F	1375	FMN	C4A-C10-N10	3.30	121.21	116.48
2	B	1375	FMN	C4A-C10-N10	3.30	121.20	116.48
2	F	1375	FMN	C4-N3-C2	-3.24	119.88	125.64
2	B	1375	FMN	C10-C4A-N5	-3.11	118.45	124.81
2	D	1375	FMN	C9A-C5A-N5	-3.06	119.21	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1375	FMN	C4-N3-C2	-3.05	120.23	125.64
2	A	1375	FMN	C4-N3-C2	-3.01	120.30	125.64
2	H	1375	FMN	C4-N3-C2	-2.87	120.54	125.64
2	D	1375	FMN	C4-N3-C2	-2.87	120.55	125.64
2	C	1375	FMN	C10-C4A-N5	-2.86	118.97	124.81
2	F	1375	FMN	C10-C4A-N5	-2.84	119.01	124.81
2	E	1375	FMN	C4A-C4-N3	2.83	120.47	113.25
2	E	1375	FMN	C4-N3-C2	-2.82	120.63	125.64
2	D	1375	FMN	C4A-C4-N3	2.76	120.27	113.25
2	D	1375	FMN	C4A-C10-N10	2.75	120.42	116.48
2	A	1375	FMN	C4A-C4-N3	2.73	120.20	113.25
2	D	1375	FMN	C5A-C9A-N10	2.71	120.42	117.97
2	C	1375	FMN	C9A-C5A-N5	-2.66	119.63	122.45
2	H	1375	FMN	C4A-C4-N3	2.66	120.03	113.25
2	E	1375	FMN	C4A-C10-N10	2.66	120.29	116.48
2	D	1375	FMN	C10-C4A-N5	-2.63	119.44	124.81
2	F	1375	FMN	C4A-C4-N3	2.57	119.80	113.25
2	H	1375	FMN	C9A-C5A-N5	-2.47	119.83	122.45
2	A	1375	FMN	C10-C4A-N5	-2.45	119.80	124.81
2	E	1375	FMN	C10-C4A-N5	-2.44	119.83	124.81
2	D	1375	FMN	C5'-C4'-C3'	-2.41	107.66	112.22
2	C	1375	FMN	C4A-C4-N3	2.37	119.30	113.25
2	G	1375	FMN	C4A-C4-N3	2.37	119.30	113.25
2	C	1375	FMN	C4-N3-C2	-2.36	121.45	125.64
2	B	1375	FMN	C4A-C4-N3	2.32	119.16	113.25
2	G	1375	FMN	C4A-C10-N10	2.31	119.79	116.48
2	A	1375	FMN	C4A-C10-N10	2.31	119.79	116.48
2	B	1375	FMN	C4A-C10-N1	-2.31	118.94	124.59
2	G	1375	FMN	C10-C4A-N5	-2.29	120.13	124.81
2	H	1375	FMN	C10-C4A-N5	-2.28	120.16	124.81
2	H	1375	FMN	O4-C4-C4A	-2.25	120.58	126.53
2	E	1375	FMN	C10-N1-C2	2.25	121.71	116.85
2	A	1375	FMN	O4-C4-C4A	-2.24	120.62	126.53
2	H	1375	FMN	C4A-C10-N10	2.23	119.68	116.48
2	D	1375	FMN	C4-C4A-N5	2.23	121.29	118.21
2	G	1375	FMN	C4-N3-C2	-2.20	121.73	125.64
2	E	1375	FMN	O4-C4-C4A	-2.18	120.78	126.53
2	A	1375	FMN	C4A-C10-N1	-2.15	119.32	124.59
2	E	1375	FMN	C4-C4A-N5	2.13	121.14	118.21
2	F	1375	FMN	C4A-C10-N1	-2.11	119.41	124.59
2	A	1375	FMN	C10-N1-C2	2.11	121.42	116.85
2	F	1375	FMN	C4-C4A-N5	2.09	121.10	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1375	FMN	C4A-C10-N1	-2.09	119.46	124.59
2	C	1375	FMN	C4-C4A-N5	2.08	121.07	118.21
2	E	1375	FMN	C4A-C10-N1	-2.07	119.51	124.59
2	D	1375	FMN	O4-C4-C4A	-2.02	121.19	126.53
2	E	1375	FMN	C9A-C5A-N5	-2.00	120.33	122.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1375	FMN	C1'-C2'-C3'-C4'
2	E	1375	FMN	O2'-C2'-C3'-C4'
2	F	1375	FMN	O2'-C2'-C3'-C4'
2	D	1375	FMN	C4'-C5'-O5'-P
2	H	1375	FMN	C4'-C5'-O5'-P
2	C	1375	FMN	C4'-C5'-O5'-P
2	E	1375	FMN	C4'-C5'-O5'-P
2	B	1375	FMN	C2'-C3'-C4'-O4'
2	G	1375	FMN	C4'-C5'-O5'-P
2	B	1375	FMN	C2'-C3'-C4'-C5'
2	A	1375	FMN	C4'-C5'-O5'-P
2	B	1375	FMN	O3'-C3'-C4'-C5'
2	E	1375	FMN	O2'-C2'-C3'-O3'
2	F	1375	FMN	C4'-C5'-O5'-P
2	B	1375	FMN	C4'-C5'-O5'-P
2	F	1375	FMN	C2'-C3'-C4'-O4'

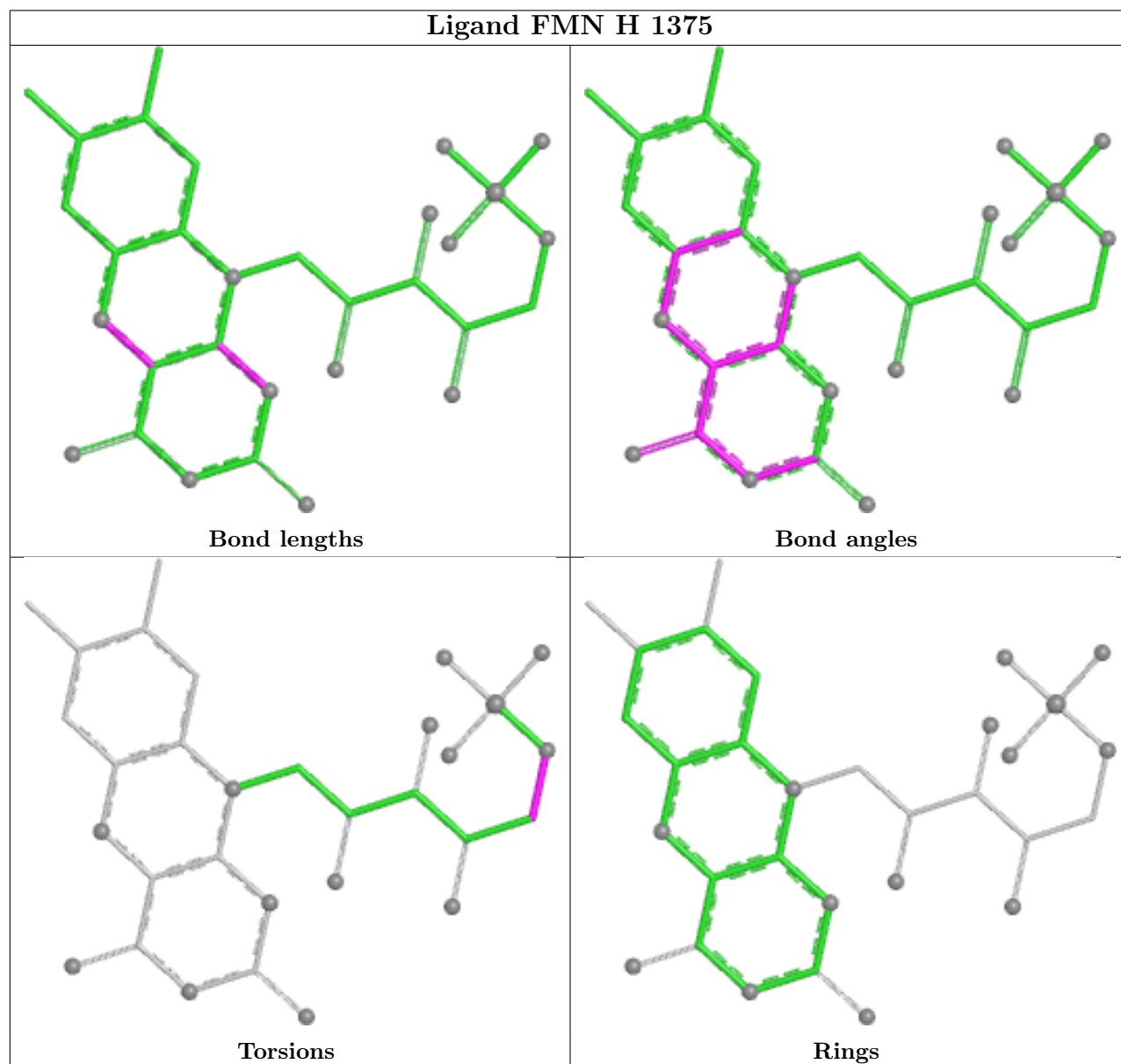
There are no ring outliers.

2 monomers are involved in 2 short contacts:

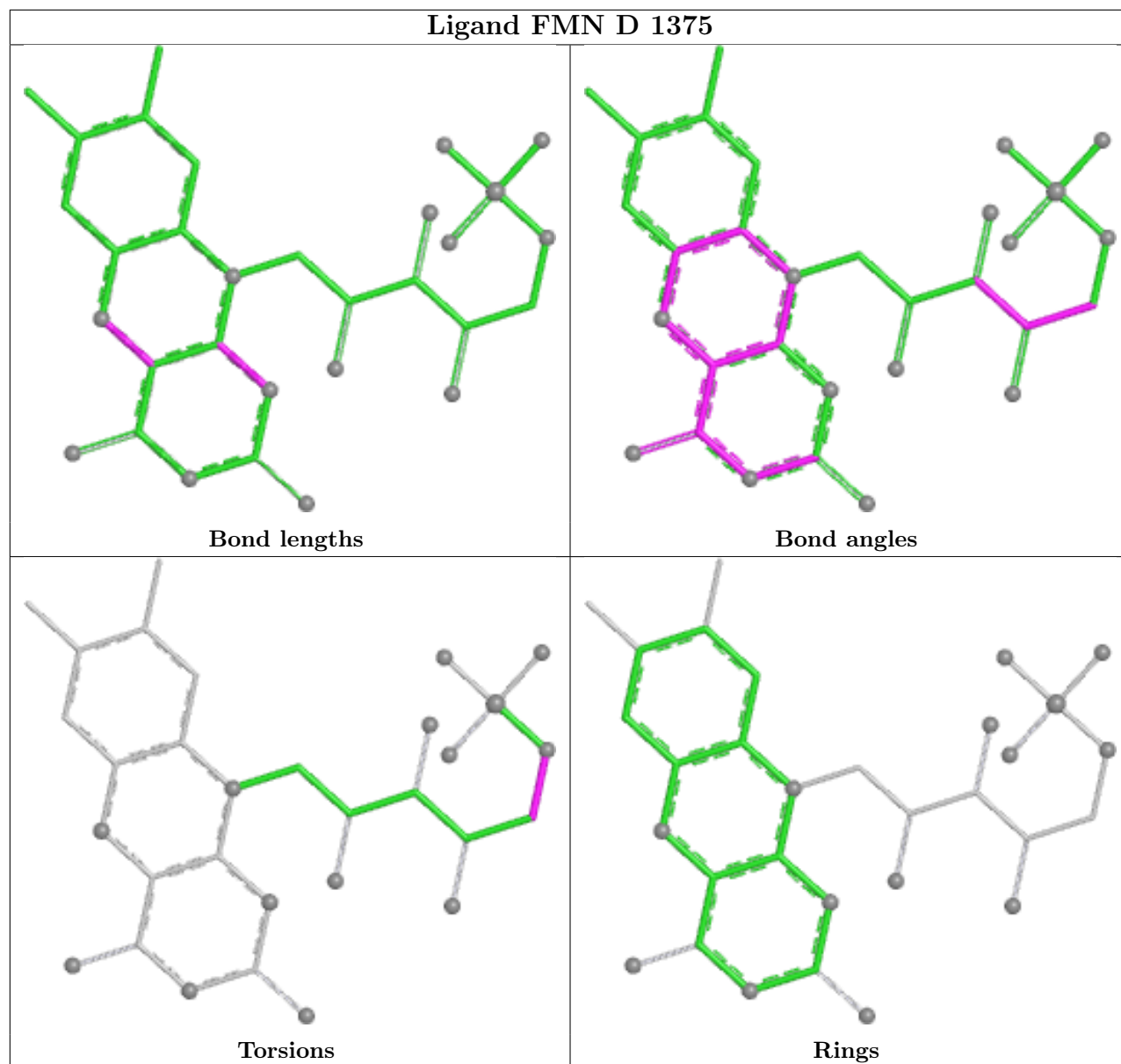
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1375	FMN	1	0
2	G	1375	FMN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

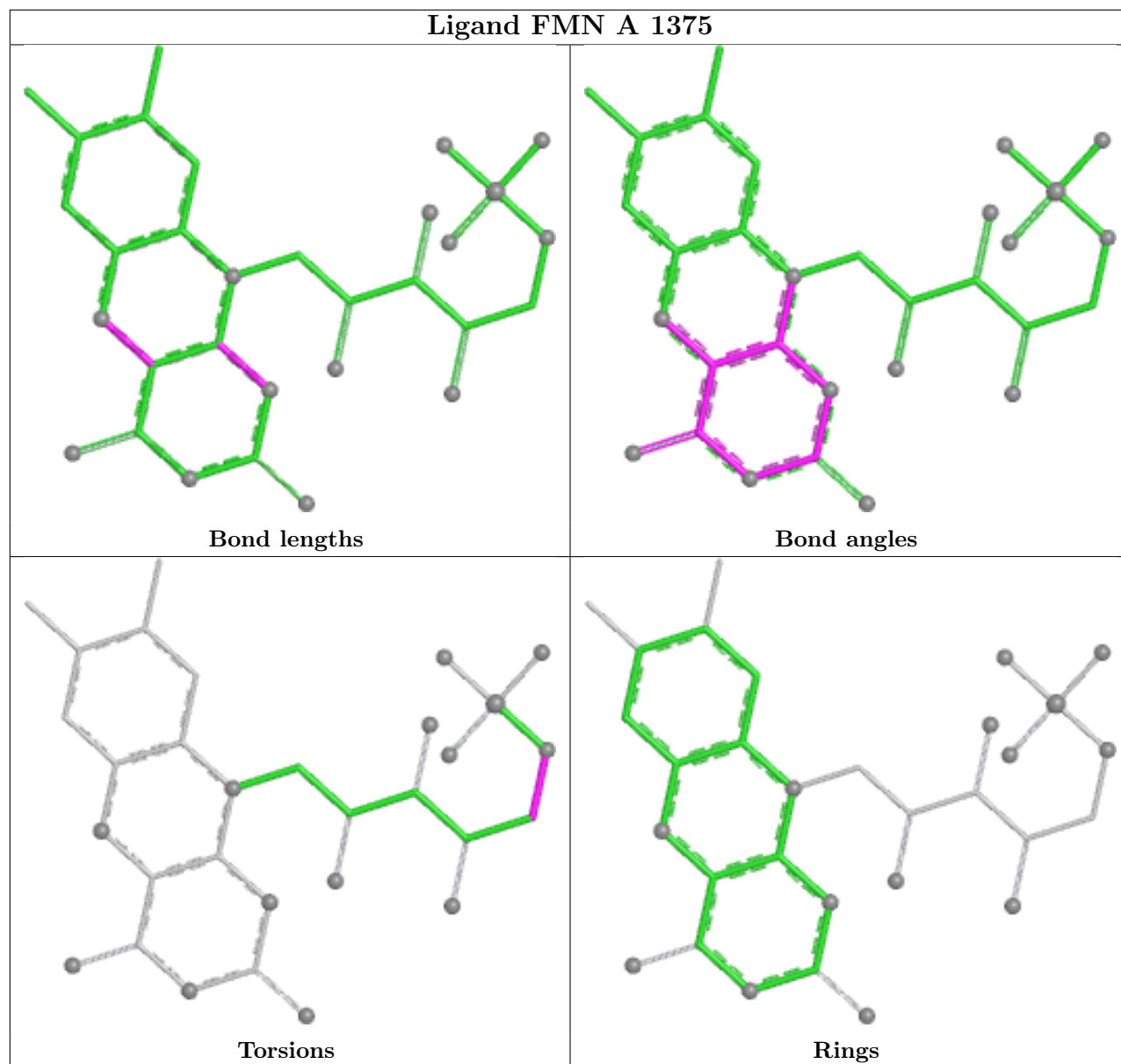
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



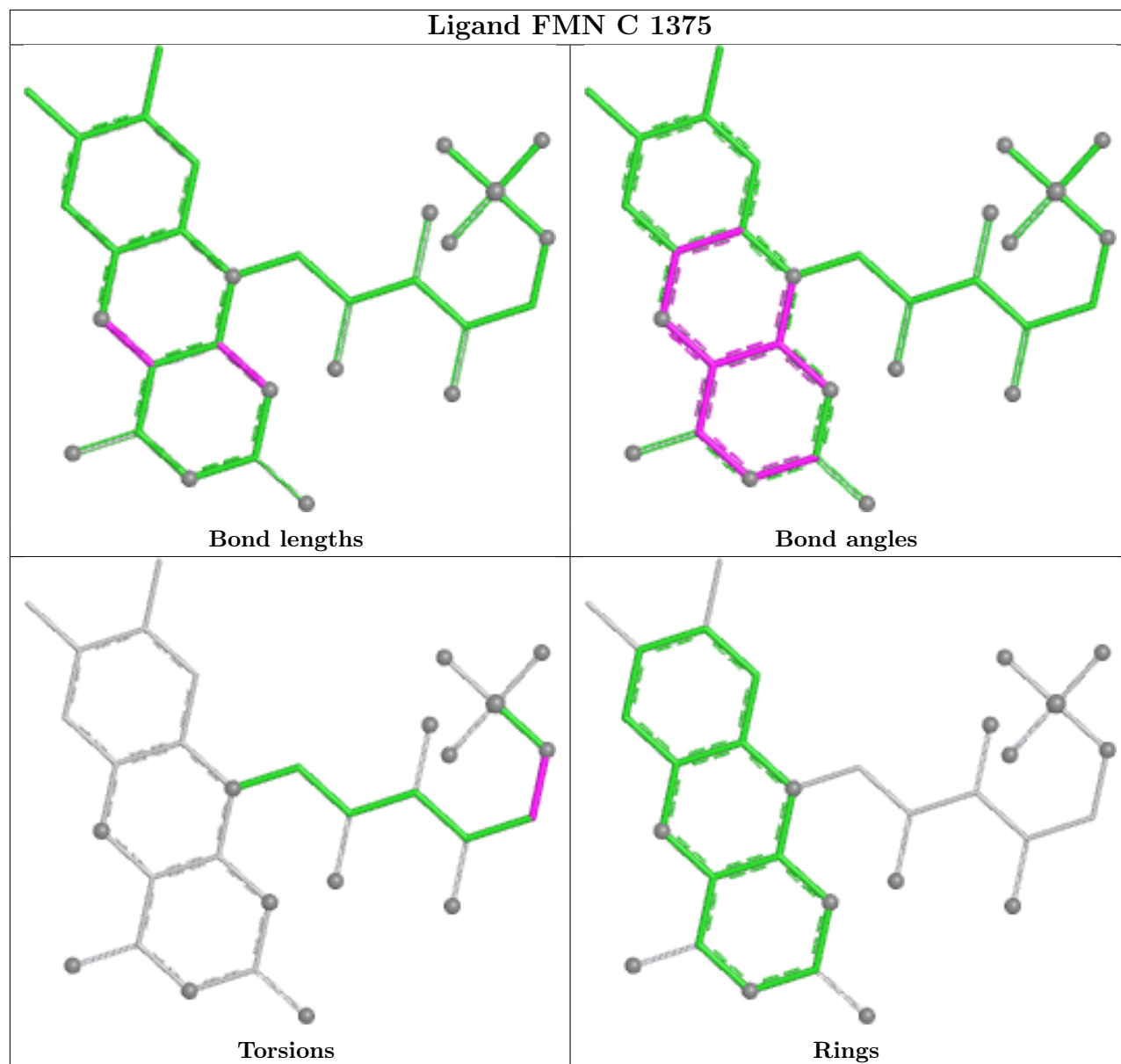
Ligand FMN D 1375



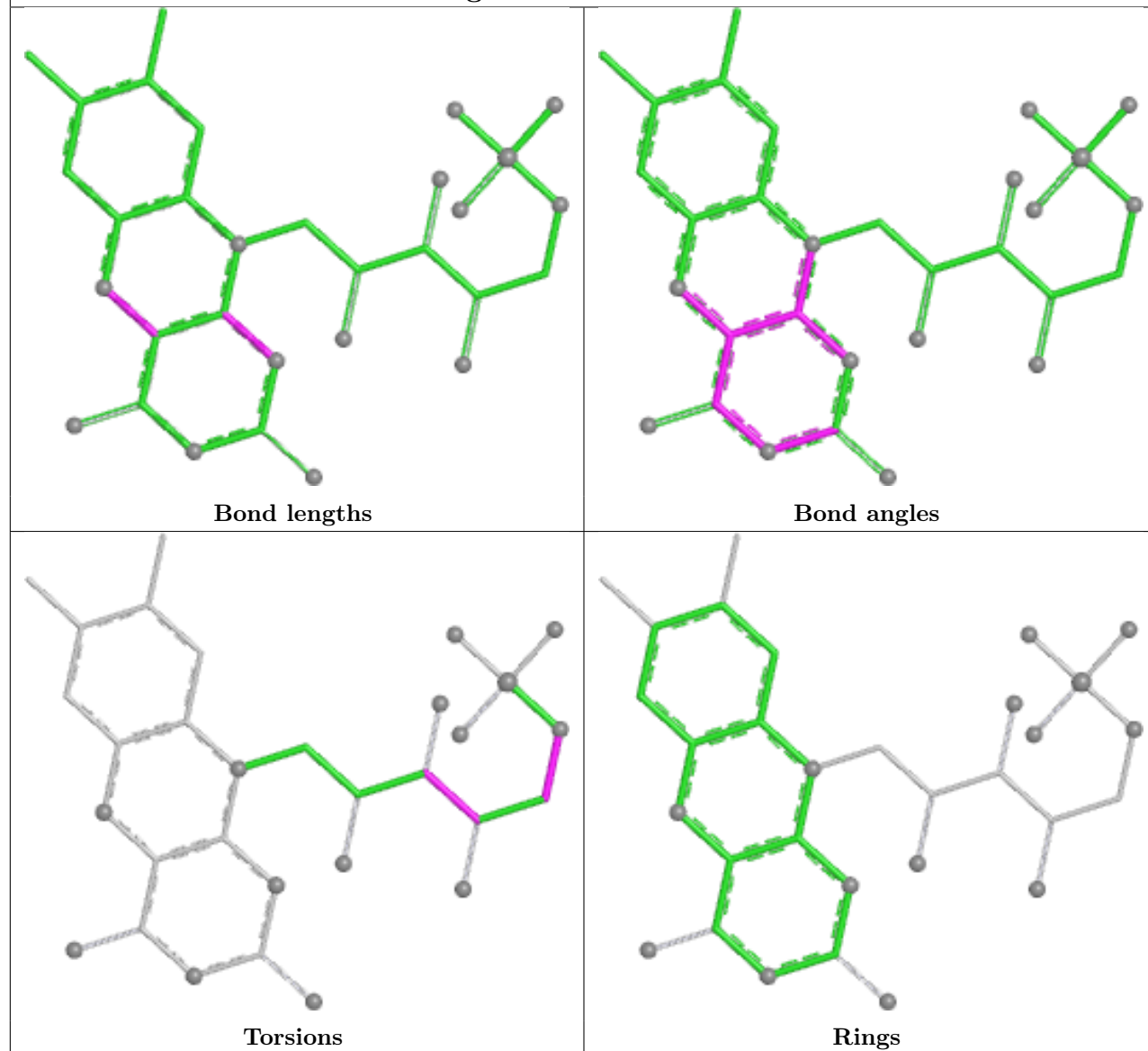
Ligand FMN A 1375



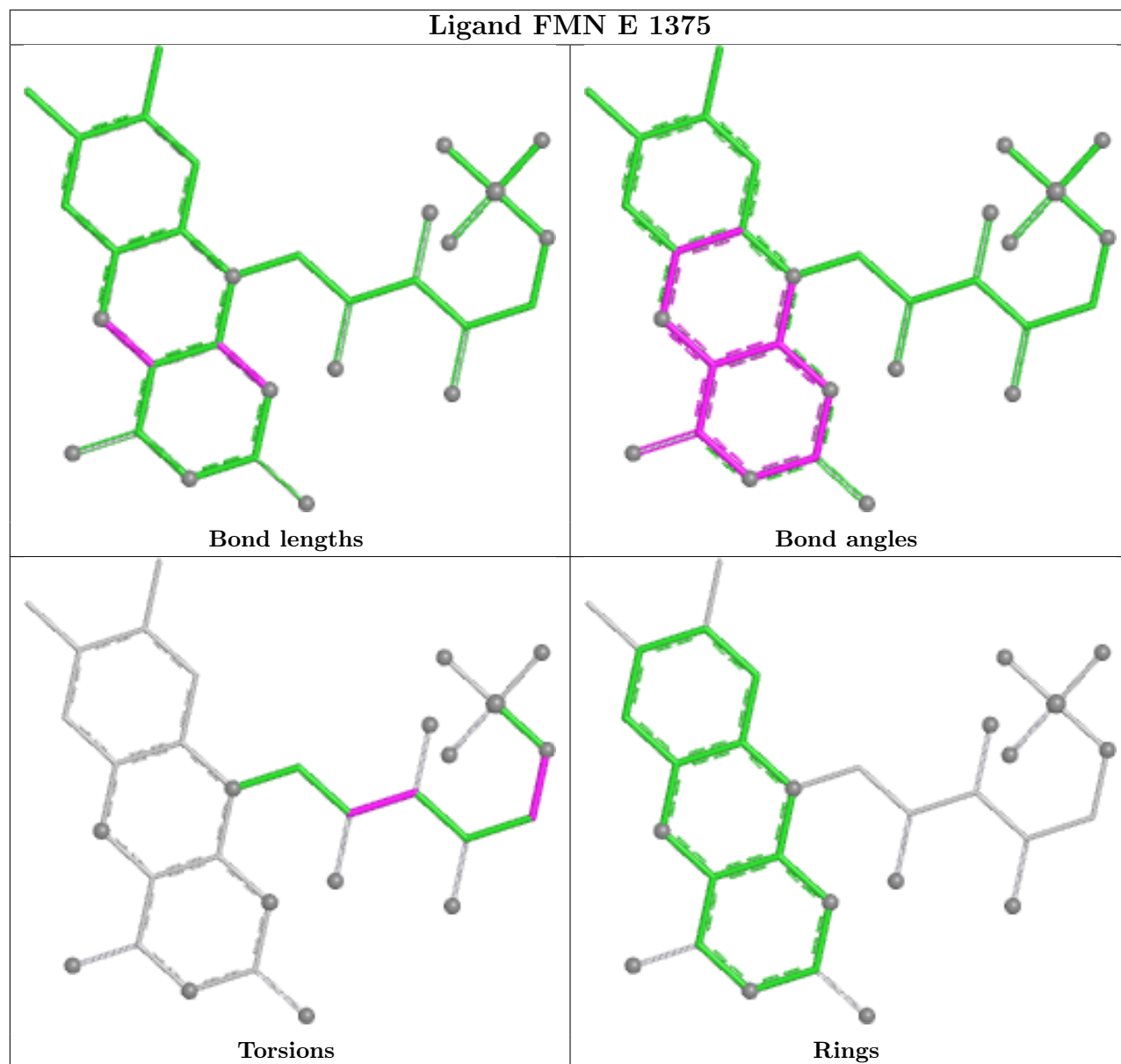
Ligand FMN C 1375



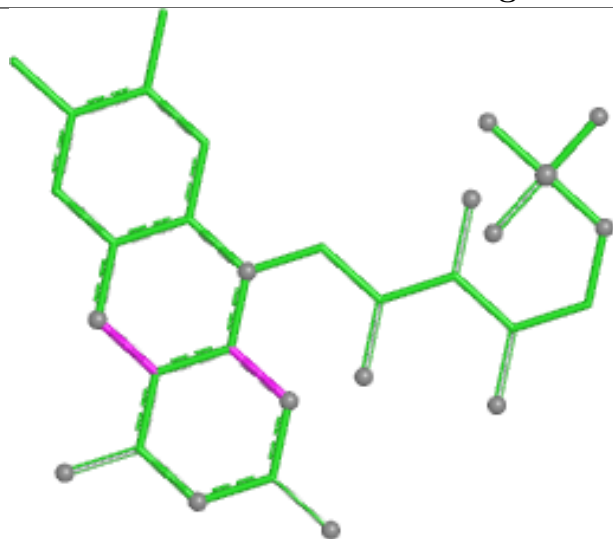
Ligand FMN B 1375



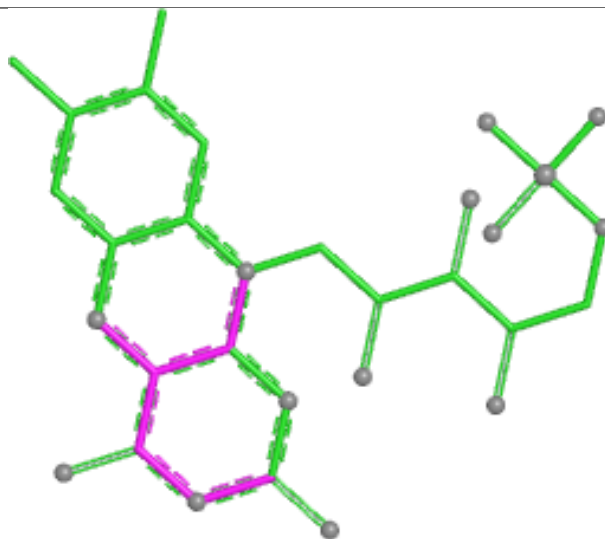
Ligand FMN E 1375



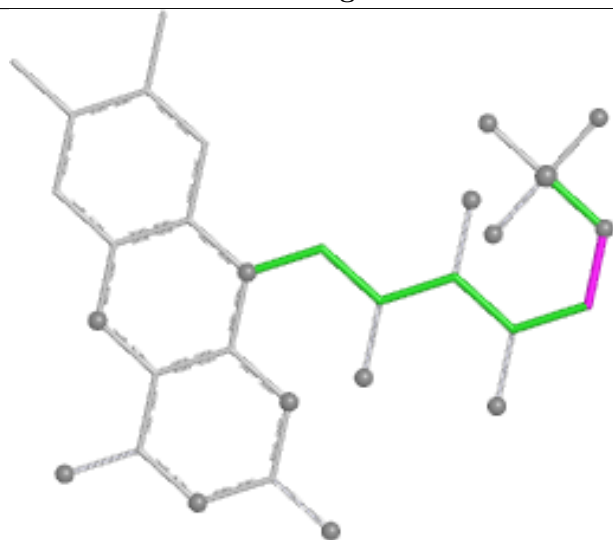
Ligand FMN G 1375



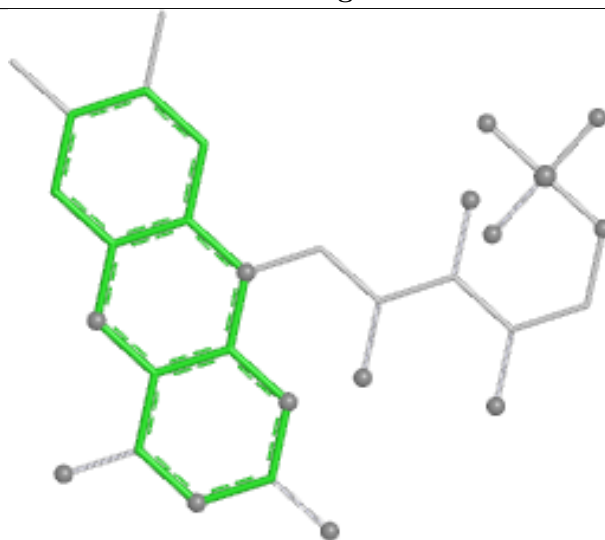
Bond lengths



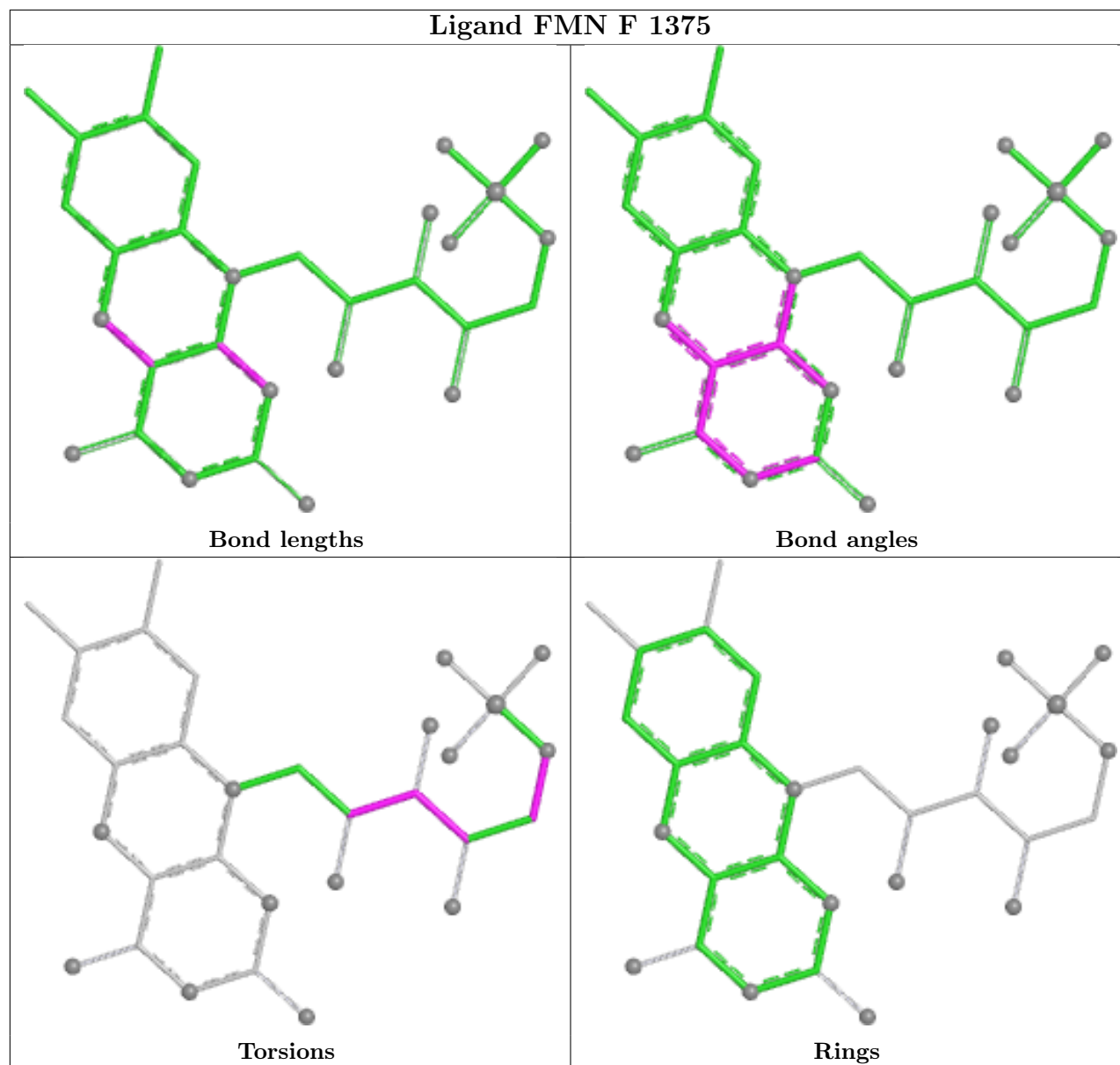
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	370/374 (98%)	-0.58	0 100 100	2, 9, 20, 27	0
1	B	367/374 (98%)	-0.46	0 100 100	3, 11, 21, 25	0
1	C	368/374 (98%)	-0.58	1 (0%) 90 91	2, 8, 19, 28	0
1	D	353/374 (94%)	-0.21	5 (1%) 73 75	3, 14, 34, 49	0
1	E	367/374 (98%)	-0.17	3 (0%) 82 84	5, 17, 31, 40	0
1	F	357/374 (95%)	-0.39	0 100 100	3, 12, 24, 43	0
1	G	367/374 (98%)	-0.34	1 (0%) 90 91	4, 13, 25, 29	0
1	H	348/374 (93%)	-0.41	1 (0%) 90 91	3, 11, 26, 35	0
All	All	2897/2992 (96%)	-0.39	11 (0%) 88 90	2, 12, 26, 49	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	ILE	3.5
1	H	197	ILE	3.4
1	D	216	GLY	2.8
1	G	82	GLY	2.7
1	E	128	THR	2.4
1	D	217	ALA	2.4
1	D	198	VAL	2.4
1	E	9	ASN	2.2
1	E	95	ALA	2.1
1	C	228	GLU	2.1
1	D	218	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

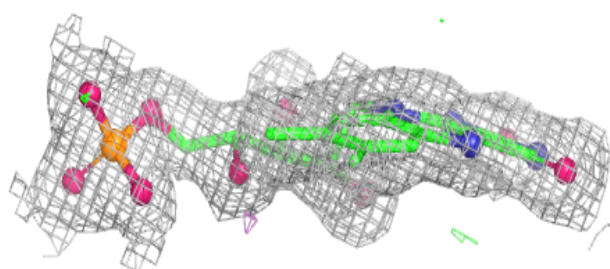
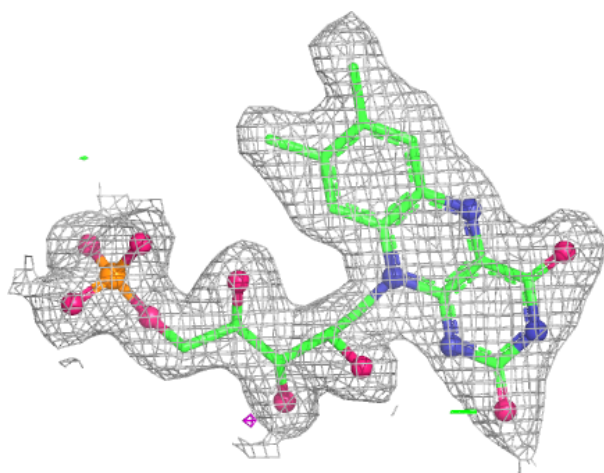
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	C	1375	31/31	0.96	0.05	2,5,7,8	0
2	FMN	B	1375	31/31	0.97	0.05	5,7,9,9	0
2	FMN	A	1375	31/31	0.97	0.05	2,6,8,9	0
2	FMN	E	1375	31/31	0.97	0.05	9,11,13,13	0
2	FMN	F	1375	31/31	0.97	0.05	3,7,8,9	0
2	FMN	G	1375	31/31	0.97	0.06	5,9,11,11	0
2	FMN	H	1375	31/31	0.97	0.05	5,8,10,13	0
2	FMN	D	1375	31/31	0.98	0.04	5,8,11,12	0
3	ZN	D	1376	1/1	0.99	0.02	26,26,26,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

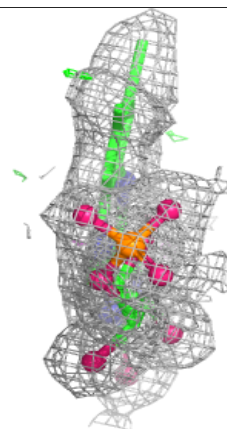
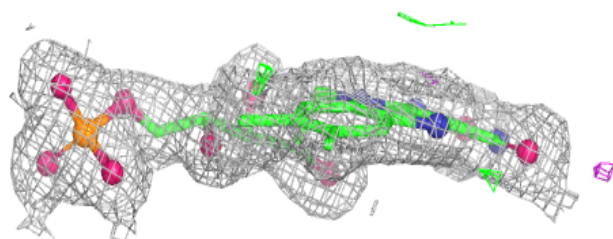
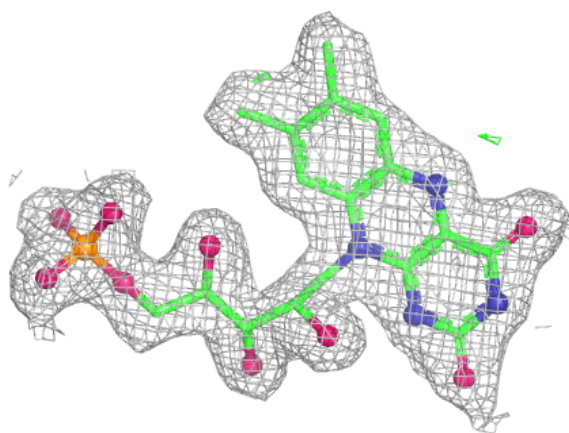
Electron density around FMN C 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



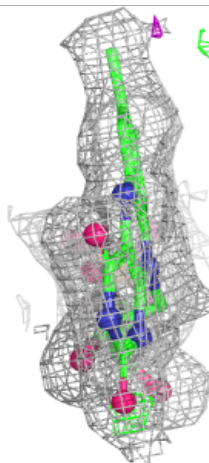
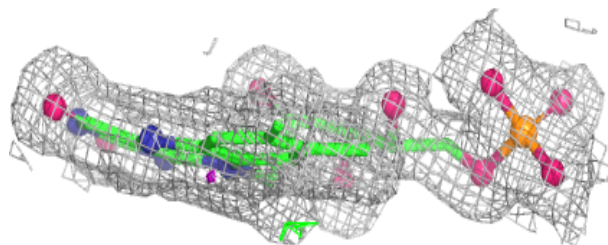
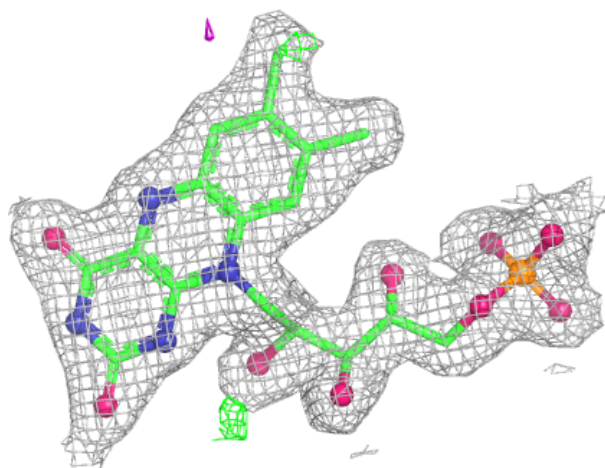
Electron density around FMN B 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



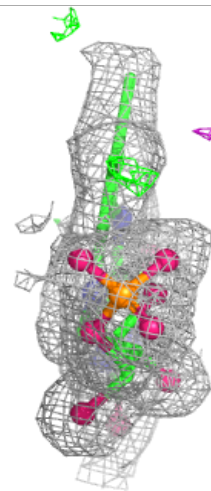
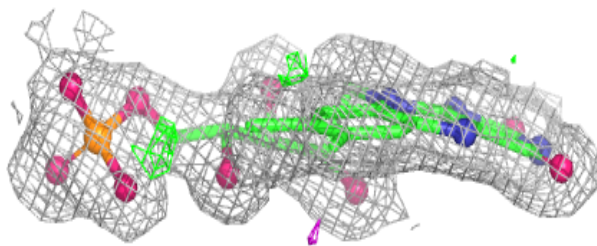
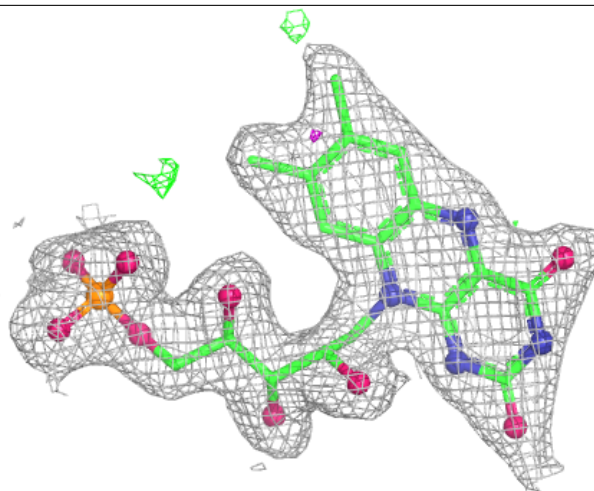
Electron density around FMN A 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



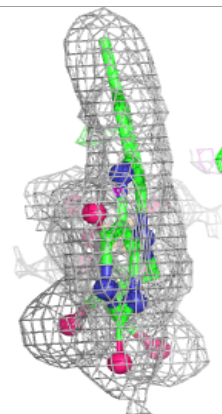
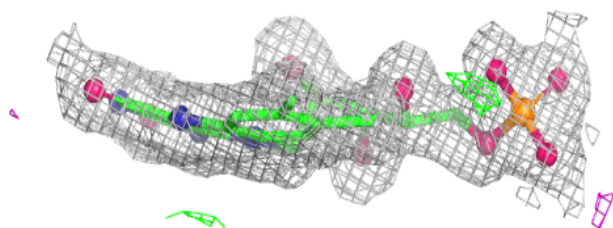
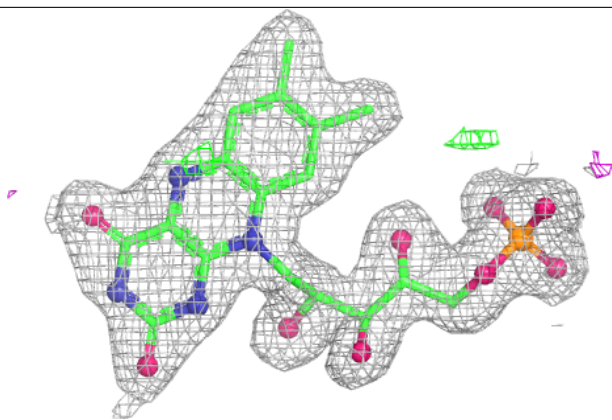
Electron density around FMN E 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

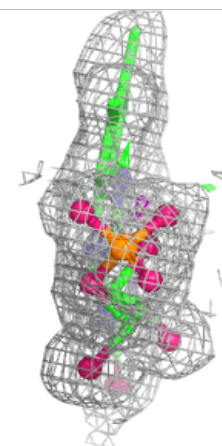
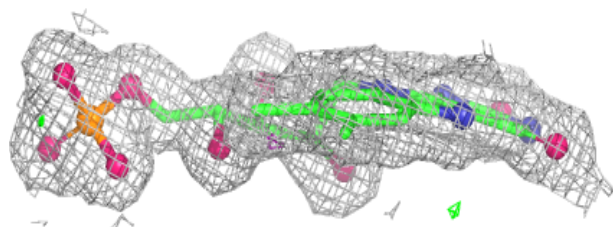
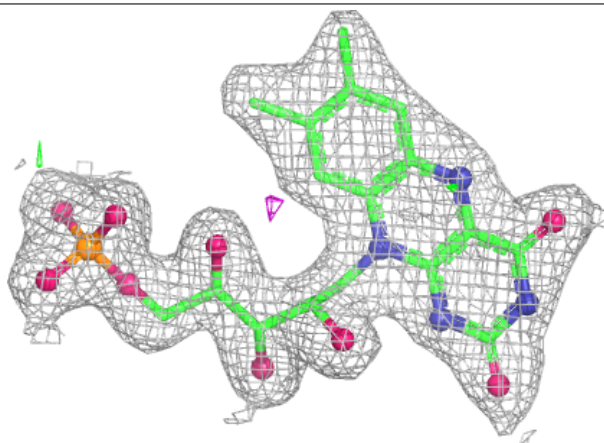


Electron density around FMN F 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

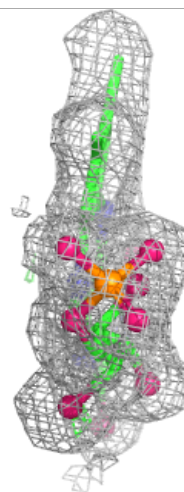
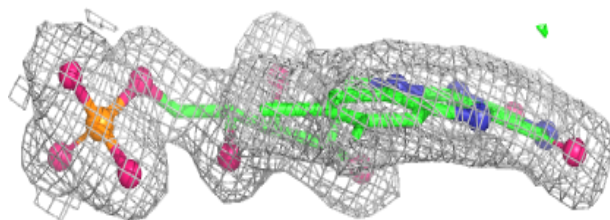
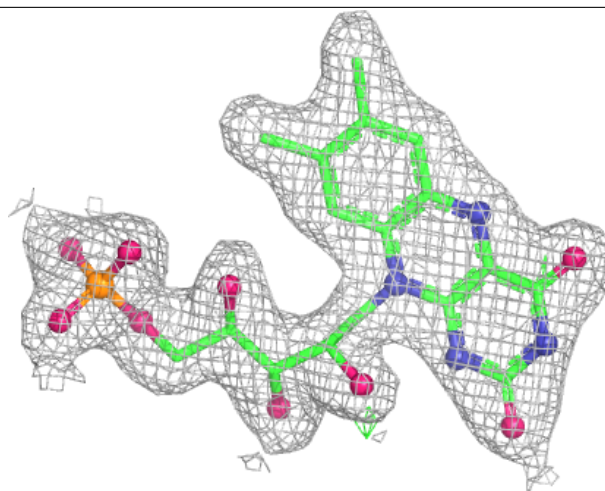
**Electron density around FMN G 1375:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



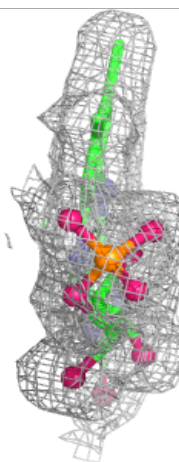
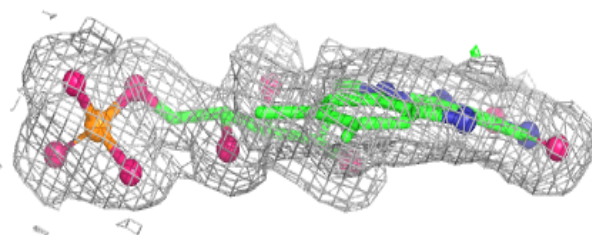
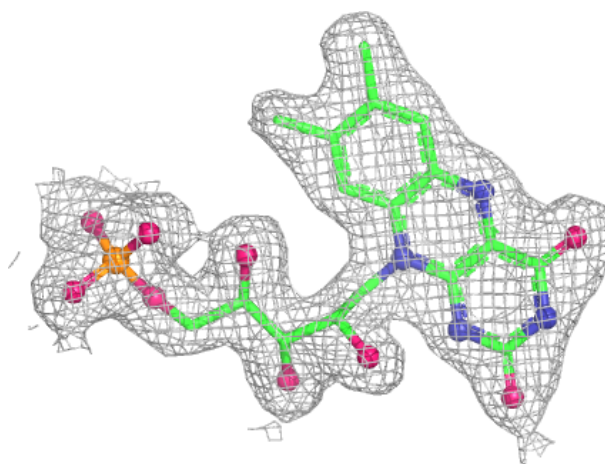
Electron density around FMN H 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN D 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.